Homework 5 Selected Solutions
APPM/MATH 4650 Fall '20 Numerical Analysis

Due date: Saturday, October 10, before midnight, via Gradescope. **Instructor**: Prof. Becker
Theme: Finite differences

solutions version 12/9/2020

Problem 1: 3-point finite difference formulas for unequispaced grid Consider a 3-point finite difference formula using the grid values $\{x, x+h, x+3h\}$. We'll assume that the function f we apply the formula to is in $C^3([x-1, x+1])$.

a) Using these nodes, our finite difference formula to approximate $f'(x)$ has the form

$$\frac{Af(x) + Bf(x+h) + Cf(x+3h)}{h}.$$

Using Taylor expansion, determine the values of A, B and C that are needed to make this an $O(h^2)$ accurate approximation of $f'(x)$. *Note:* If you need to solve a linear system, you may do this via a computer, but your final answers should be exact (like 1/3 not 0.3333).

Solution:

Taylor expanding, we get

$$\begin{aligned}
&\frac{A}{h}f(x)\\
&+\frac{B}{h}\Big(f(x) + hf'(x) + h^2/2f''(x) + O(h^3)\Big)\\
&+\frac{C}{h}\Big(f(x) + 3hf'(x) + 9h^2/2f''(x) + O(h^3)\Big)\\
&= h^{-1}\left(\underbrace{(A+B+C)}_{0}f(x) + \underbrace{(B+3C)}_{1}hf'(x) + \underbrace{(B+9C)}_{0}h^2/2f''(x) + O(h^3)\right)
\end{aligned}$$

meaning we want to solve the system of linear equations

$$\begin{bmatrix} A & B & C \\ 0 & B & 3C \\ 0 & B & 9C \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

which we write as

$$\begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 3 \\ 0 & 1 & 9 \end{bmatrix}\begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

and solve this by hand or via a computer (e.g., in Matlab, the backslash operator `\` or in Python `numpy.linalg.solve`). If using a computer, to round to rational coefficients, in Matlab use `rat( ... )` and in Python there are several ways, like `import sympy` then `sympy.nsimplify( ... )` (or see here for other ideas). Be aware that this is just rounding to a nearby rational, so then you need to plug in the rational into the equation to verify it's indeed the exact answer. Doing this gives the answer $\boxed{[A, B, C] = [-4/3, 3/2, -1/6] = [-4, 3, -1]/6}$.

Note that the last equation is not necessary if we just want a method that is $O(h)$, but since we want an $O(h^2)$ method we need to include that last equation.

Throughout this problem we are using the fact that since $f \in C^3([x-1, x+1])$, this means f''' is bounded (by the extreme value theorem), which is why we say that a term like $f'''(\xi)h^3 = O(h^3)$.

Also note that our coefficient matrix has determinant 6, meaning it is invertible, so the solution we found is unique. More on this in part (c).

b) Repeat the above exercise but this time find the coefficients A, B and C by constructing the Lagrange interpolating polynomial $p(x)$ and differentiating p at x. *Hint:* to simplify the derivation, you can assume without loss of generality that $x = 0$, since only the *spacing* between the nodes matters.

Solution:

Without loss of generality, let $x = 0$, so our nodes are $\{x_0 = 0, x_1 = h, x_2 = 3h\}$. The interpolating polynomial is

$$p(x) = f(0)\ell_0(x) + f(h)\ell_1(x) + f(3h)\ell_2(x)$$

where

$$\begin{aligned}
\ell_0(x) &= \frac{(x-h)(x-3h)}{(-h)(-3h)} = \frac{1}{3h^2}\left(x^2 - 4hx + 3h^2\right) \\
\ell_1(x) &= \frac{(x)(x-3h)}{(h)(h-3h)} = -\frac{1}{2h^2}\left(x^2 - 3hx\right) \\
\ell_2(x) &= \frac{(x)(x-h)}{(3h)(3h-h)} = \frac{1}{6h^2}\left(x^2 - hx\right)
\end{aligned}$$

since the formula for the i^{th} Lagrange polynomial of degree n is $\ell_i(x) = \prod_{j=0, j\neq i}^{n} \frac{x - x_j}{x_i - x_j}$. We calculate

$$\begin{aligned}
\ell_0'(x) &= \frac{1}{3h^2}(2x - 4h) \quad \text{so} \quad \ell_0'(0) = -\frac{4}{3h} \\
\ell_1'(x) &= -\frac{1}{2h^2}(2x - 3h) \quad \text{so} \quad \ell_1'(0) = \frac{3}{2h} \\
\ell_2'(x) &= \frac{1}{6h^2}(2x - h) \quad \text{so} \quad \ell_2'(0) = -\frac{1}{6h}.
\end{aligned}$$

Then we find our estimate for $f'(0)$ by computing $p'(0)$, which is

$$p'(0) = f(0)\ell_0'(0) + f(h)\ell_1'(0) + f(3h)\ell_2'(0) = \boxed{\frac{\frac{-4}{3}f(0) + \frac{1}{3}f(h) - \frac{1}{6}f(3h)}{h}}$$

so we see that this is the same formula we found in part a) [after we change the $x = 0$ back to a generic x].

c) If we want an $O(h^2)$ approximation, are the choices for A, B and C unique? If we only want our formula to be an $O(h)$ approximation, now are the choices for A, B and C unique?

Solution:

Yes, they are unique because as we saw from part (a), if we want to cancel the $O(h)$ term and thus have an $O(h^2)$ approximation, we must solve that linear system, and the coefficient matrix was invertible (since its determinant was nonzero), so there's a unique solution.

If we only want an $O(h)$ approximation, then we only use the first two rows of the matrix, and the matrix is no longer square, so either there are no solutions or an entire subspace (hence an infinite nubmer) of solutions. Since we know that the full 3×3 system had a solution, this 2×3 system also has a solution, hence we have an infinite number of solutions.

Interestingly, the interpolating polynomial method gave us the "best" solution, e.g., of the infinite $O(h)$ formulas, it gave us the only $O(h^2)$ formula.

d) Now let's use these nodes to make a finite difference formula to approximate $f''(x)$, using the form
$$\frac{Af(x) + Bf(x+h) + Cf(x+3h)}{h^2}.$$
Using Taylor expansion, find the values of A, B and C to approximate $f''(x)$ such that the error in the approximation goes to 0 as $h \to 0$.

Solution:

Just as in part (a), we Taylor expand, getting

$$\begin{aligned}
&\frac{A}{h^2} f(x) \\
&+\frac{B}{h^2}\Big(f(x) + hf'(x) + h^2/2f''(x) + O(h^3)\Big) \\
&+\frac{B}{h^2}\Big(f(x) + 3hf'(x) + 9h^2/2f''(x) + O(h^3)\Big) \\
&= h^{-2}\left(\underbrace{(A+B+C)}_{0} f(x) + \underbrace{(B+3C)}_{0} hf'(x) + \underbrace{(B+9C)}_{2} h^2/2f''(x) + O(h^3)\right)
\end{aligned}$$

meaning we want to solve the system of linear equations

$$\begin{bmatrix} A & B & C \\ 0 & B & 3C \\ 0 & B & 9C \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}$$

which we write as

$$\begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 3 \\ 0 & 1 & 9 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}$$

and solve this by hand or via a computer. Everything is the same as in part (a) except now we have a different RHS; in particular, the matrix is invertible, and there is only one solution. Don't forget that the RHS has a 2 in the lowest entry, not a 1 (this comes from the 1/2 we need to cancel in the Taylor series). Note that our approximation is now just $O(h)$, since we divide the $O(h^3)$ error by h^2 instead of just h. We don't have enough degrees of freedom to cancel the $O(h)$ error term, though we could do that if we had a 4-point stencil.

Actually solving the system gives $[A, B, C] = \boxed{[2/3, -1, 1/3]}$.

e) Repeat the above exercise but this time find the coefficients A, B and C by constructing the Lagrange interpolating polynomial $p(x)$ and differentiating p twice at x.

Solution:

Very similar to part (b), we calculate

$$\begin{aligned}
\ell_0'(x) &= \frac{1}{3h^2}(2x - 4h) \quad \text{so} \quad \ell_0''(x) = \frac{2}{3h^2} \\
\ell_1'(x) &= -\frac{1}{2h^2}(2x - 3h) \quad \text{so} \quad \ell_1''(x) = -\frac{1}{h^2} \\
\ell_2'(x) &= \frac{1}{6h^2}(2x - h) \quad \text{so} \quad \ell_2''(x) = \frac{1}{3h^2}.
\end{aligned}$$

Name	Order	Node location						
		$-3h$	$-2h$	$-h$	0	h	$2h$	$3h$
2-pt forward diff.	1	0	0	0	-1	1	0	0
3-pt forward diff.	2	0	0	0	$-3/2$	$4/2$	$-1/2$	0
4-pt forward diff.	3	0	0	0	$-11/6$	$18/6$	$-9/6$	$2/6$
3-pt centered diff.	2	0	0	$-1/2$	0	$1/2$	0	0
5-pt centered diff.	4	0	$1/12$	$-8/12$	0	$8/12$	$-1/12$	0
7-pt centered diff.	6	$-1/60$	$9/60$	$-45/60$	0	$45/60$	$-9/60$	1

Table 1: Forward and centered difference formula to approximate the first derivative

As before, we approximate $f''(0)$ using $p''(0)$, and

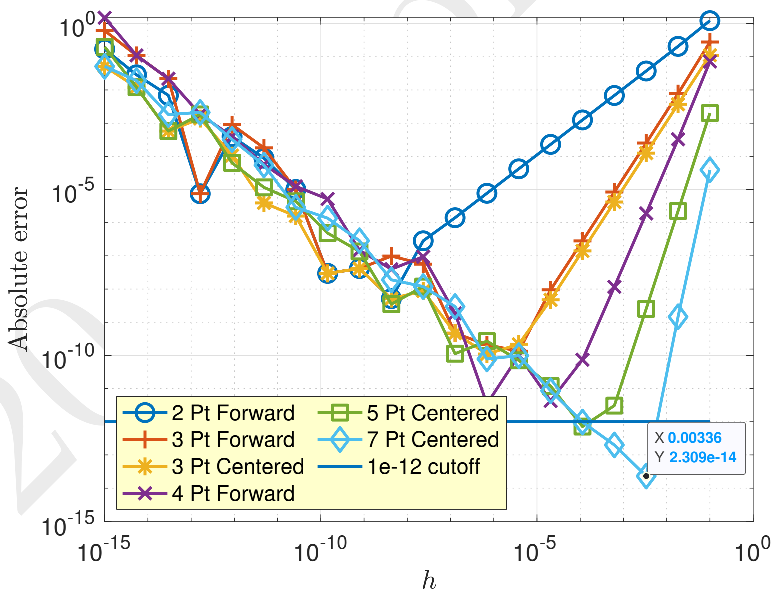
$$p''(0) = f(0)\frac{2}{3h^2} - f(h)\frac{1}{h^2} + f(3h)\frac{1}{3h^2}$$

so putting this into the form of problem (d), we again find $[A, B, C] = \boxed{[2/3, -1, 1/3]}$.

Problem 2: Let $f(x) = e^{3x}$ and $x = 0.3$. Approximate $f'(0.3)$ to within 10^{-12} absolute error using one of the finite difference rules in Table 1. Report which rule you used and what stepsize h. *Optional but recommended:* plot the errors for each method as a function of the stepsize.

Solution:

We plot the errors as a function of h for all the stepsizes in the plot:



Your plot may look slightly different depending on exactly which h values you used. We can see from our plot that using the 7 point centered difference method with a stepsize of $h = 0.00336$ gives us an error of $2.3 \cdot 10^{-14}$. The stepsize you find might be a bit different, but something in the range of $[10^{-4}, 10^{-2}]$. You might be able to get error less than 10^{-12} using the 5 point centered difference formula if you get a good choice of h, so either 5 or 7 point centered difference formulas are OK.

The whole point of this exercise is that we *cannot* just take $h \to 0$, as then roundoff error dominates. We discussed this in the Ch4_FiniteDifferences.ipynb demo.

Matlab code to make the plot is below.

```
f       = @(x) exp(3*x);
fprime  = @(x) 3*exp(3*x);
x   = 0.3;

labels = {}; formulas = {};
formulas{end+1} = @(h) (f(x+h)-f(x))/h;
  labels{end+1} = '2 Pt Forward';
formulas{end+1} = @(h) (-f(x+2*h)+4*f(x+h)-3*f(x))/(2*h);
  labels{end+1} = '3 Pt Forward';
formulas{end+1} = @(h) (f(x+h)-f(x-h))/(2*h);
  labels{end+1} = '3 Pt Centered';
formulas{end+1} = @(h) (2*f(x+3*h)-9*f(x+2*h)+18*f(x+h)-11*f(x))/(6*h);
  labels{end+1} = '4 Pt Forward';
formulas{end+1} = @(h) (-f(x+2*h)+8*f(x+h)-8*f(x-h)+f(x-2*h))/(12*h);
  labels{end+1} = '5 Pt Centered';
formulas{end+1} = @(h) (f(x+3*h) - 9*f(x+2*h)+45*f(x+h)-45*f(x-h)+9*f(x-2*h)-f(x
    -3*h))/(60*h);
  labels{end+1} = '7 Pt Centered';

hGrid   = logspace(-1,-15,20);
errors  = zeros( length(formulas), length(hGrid) );
for i = 1:length(hGrid)
    h   = hGrid(i);
    for j = 1:length(formulas)
        errors(j,i) = abs( fprime(x) - formulas{j}(h) );
    end
end

% Do the plotting
hndl = loglog( hGrid, errors,'o-','linewidth',2,'markersize',12);
markers = 'o+*xsd^v><';
for j=1:length(hndl), hndl(j).Marker=markers(j);end
grid on; set(gca,'FontSize',16);
hndl=legend(labels,'location','southwest','box','on','NumColumns',2);
hndl.Color = [255, 255, 204]/255;
line([hGrid(end),hGrid(1)], 1e-12*[1,1],'linewidth',2,'DisplayName',...
    '1e-12 cutoff');
xlabel('$h$','interpreter','latex');
ylabel('Absolute error','interpreter','latex');
export_fig HW5_Problem2 -pdf -transparent % https://github.com/altmany/export_fig
```

Problem 3: Consider the 3-pt centered difference formula $f'(x) \approx \frac{f(x+h)-f(x-h)}{2h}$ which is $O(h^2)$. Suppose we numerically calculate $f(x+h)$ with error bounded by ϵ, and similarly for $f(x-h)$, and suppose the truncation error is bounded by Mh^2. In particular, we are supposing we can numerically compute $\frac{f(x+h)-f(x-h)}{2h}$ up to an error $2\epsilon/h$ [we assume $h > 0$, otherwise we would write this as $2\epsilon/|h|$), and that $|f'(x) - \frac{f(x+h)-f(x-h)}{2h}| \le Mh^2$. That is, the output of our numerical implementation of the formula, which we'll call δ, is

$$|\delta - f'(x)| \le 2\epsilon/h + Mh^2.$$

Find the value of h that minimizes this error bound, as well as reporting the resulting error bound.

Solution:

Let $g(h) = 2\epsilon/h + Mh^2$, and we want to minimize g over all $h > 0$. This function is differentiable for all $h > 0$, and we can exclude $h = 0$ since $g(0) = \infty$, and can also exclude $h \to \infty$ since $\lim_{h\to\infty} g(h) = \infty$.. Thus we only need to check the critical points of g, i.e., where $g'(h) = 0$. Since $g'(h) = -2\epsilon/h^2 + 2Mh$, we solve $2\epsilon/h^2 = 2Mh$, and hence get $\boxed{h = \left(\frac{\epsilon}{M}\right)^{1/3}}$, and evaluating g at this point gives $g\left(\left(\frac{\epsilon}{M}\right)^{1/3}\right) = 2\epsilon/\left(\frac{\epsilon}{M}\right)^{1/3} + M\left(\frac{\epsilon}{M}\right)^{2/3} = 2\epsilon^{2/3}M^{-1/3} + \epsilon^{2/3}M^{-1/3} = \boxed{3\epsilon^{2/3}M^{1/3}}$.

Problem 4: Misc. questions

a) Consider a finite difference formula that has truncation error $C \cdot h^n \cdot f^{(n+1)}(\xi)$ for some constant C and some $\xi \in [x, x+h]$ where x is the point of interest. What can you say about the truncation error of this finite difference formula if the function f is a polynomial f of degree n or less?

Solution:

There is no truncation error, since the remainder term is 0 since $f^{(n+1)} = 0$. You can always test this numerically.

b) If we used the 3-point centered difference formula to approximate the derivative of a quadratic function, what kind of stepsize h should we use? (large? small? medium?)

Solution:

We want h large, since it doesn't matter how big h is for truncation error so there's no reason to prefer a small h, and for roundoff error purposes we want h large.

c) Denote the 3-point centered difference formula as $N_1(h)$. Apply Richardson extrapolation to N_1 to get $N_2(h)$. What is the order of accuracy of N_2? Does $N_2(2h)$ remind you of another formula?

Solution:

Because N_1 is $O(h^2)$, the formula to cancel out the h^2 term is $N_2(h) = \frac{1}{3}\left(4N_1(h/2) - N_1(h)\right)$, as was covered in the notes, so

$$\begin{aligned} N_2(h) &= \frac{1}{3}\left(\frac{4}{2h/2}\left(f(x+\frac{h}{2}) - f(x-\frac{h}{2})\right) - \frac{1}{2h}\Big(f(x+h) - f(x-h)\Big)\right) \\ &= \frac{1}{h}\left(-\frac{1}{6}f(x+h) + \frac{4}{3}f(x+\frac{h}{2}) - \frac{4}{3}f(x-\frac{h}{2}) + \frac{1}{6}f(x-h)\right) \end{aligned}$$

thus

$$\begin{aligned} N_2(2h) &= \frac{1}{2h}\left(-\frac{1}{6}f(x+2h) + \frac{4}{3}f(x+h) - \frac{4}{3}f(x-h) + \frac{1}{6}f(x-2h)\right) \\ &= \frac{1}{h}\left(-\frac{1}{12}f(x+2h) + \frac{2}{3}f(x+h) - \frac{2}{3}f(x-h) + \frac{1}{12}f(x-2h)\right) \end{aligned}$$

which is exactly the $\boxed{\text{5-point centered difference formula}}$. The formula for N_2 has order of accuracy $O(h^4)$, which you can deduce following the notes or by noting that we know the 5-point centered difference formula is order 4 (e.g., Table 1).